

Note

**The Error Analysis of the Algebraic Method
for Solving the Schrödinger Equation**

Recently [1-3], a new method was introduced in order to solve numerically the one-dimensional time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dr^2} + V(r) \psi = E\psi. \tag{1}$$

The central idea of this method is to transform the Schrödinger equation into an algebraic system of linear equations which is obtained by approximating the potential $V(r)$ with a sequence of step functions.

This algebraic method (AM) was considered by Canosa and de Oliveira [1] for the discrete spectrum of energies and by Ixaru [2, 3] for the continuum spectrum. In the paper [1], AM is said to be a first-order method, that is, the absolute error both in the eigenvalues and eigenfunctions is $O(h)$ where h is the spatial step size. This is a somewhat discouraging result and might impede the spreading of AM despite of the real advantages of this method. A more detailed analysis of the error appears accordingly very necessary. We do it in this paper. Our result is that AM is a *second-order method*. At this point we note that another formalism for solving Eq. (1) and which is related with AM was recently introduced by Gordon [4]. He discusses at large the case when the potential V is approximated in each interval by a linear function of r which fits it as well as its first derivative at the center of the interval (the line MN on Fig. 1). He claims that his method is a third-order one but, as we show at the end of this paper, it is a second-order method, i.e. it has the same accuracy as AM. The formalism of his method is, however, significantly more complicate than that of AM.

Before starting the proof we notice a very nice peculiarity of AM: the truncation error of the method is clearly separated from the computation error. That is to say, the only approximation is to replace $V(r)$ by a sequence of step functions. Once the approximate problem is obtained, it is integrated exactly except for round-off error.

The round-off error is negligible. We studied it for the potentials occurring in the penetration problem of the spontaneous alpha decay. We saw that the error is well under 0.01 % when the number of intervals is as large as 1200. Usually and

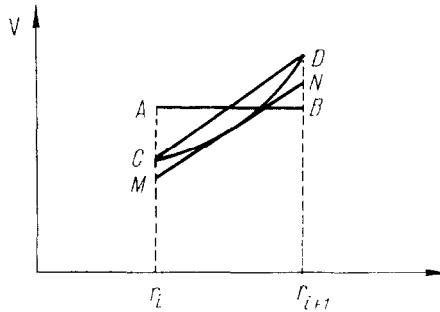


FIG. 1. The potential $V(r)$ and its two approximations: the potential \bar{V} , a constant, equal to the arithmetic mean of the extreme values of V in each interval and the chord-potential \tilde{V} . The line MN is the linear approximation of Gordon [4].

especially for the discrete spectrum, the number of intervals is very much smaller (several hundreds) and this makes the round-off error surely smaller than 0.01 %. Our problem is, therefore, reduced to the study of the truncation error.

We limit our proof to the discrete spectrum problem only. Let $I \equiv [a, b]$ be the domain of (1) whose length is L . We divide it in intervals $[r_i, r_{i+1}]$ of length h ($r_1 = a, r_q = b$ and $i = 1, 2, \dots, q - 1$) and approximate V in each interval by a constant. We denote by \bar{V} and \tilde{V} the potentials that in each interval approximate V by the arithmetic mean value and by the corresponding chord, respectively. They are represented on Fig. 1 by the lines AB and CD . The eigenvalues and eigenfunctions of (1) for the potentials \bar{V} and \tilde{V} are denoted by $\epsilon_n, \bar{\epsilon}_n$ and $\varphi_n, \bar{\varphi}_n$ respectively. As stated above, our aim is to prove that the eigenvalues ϵ_n and E_n as well as the eigenfunctions φ_n and ψ_n coincide within $O(h^2)$. As this comparison cannot be done directly, we proceed in two stages. The first stage consists in comparing ϵ_n with $\bar{\epsilon}_n$ and φ_n with $\bar{\varphi}_n$, while in the second stage one compares $\bar{\epsilon}_n$ with E_n and $\bar{\varphi}_n$ with ψ_n . The results obtained in the two stages will lead to the stated result.

In order to make the comparisons required by both stages, we use the results of the first order perturbation theory. They connect ϵ_n^1 and φ_n^1 of the potential V^1 with ϵ_n^2 and φ_n^2 of $V^2 \equiv V^1 + \Delta V$ as follows:

$$\epsilon_n^2 - \epsilon_n^1 = \langle \varphi_n^1 | \Delta V | \varphi_n^1 \rangle, \tag{2}$$

$$\varphi_n^2 - \varphi_n^1 = \sum_{k \neq n} \frac{\langle \varphi_k^1 | \Delta V | \varphi_n^1 \rangle}{\epsilon_n^1 - \epsilon_k^1} \varphi_k^1. \tag{3}$$

From these equations one sees that the size of the difference between the eigenvalues and the eigenfunctions of the unperturbed and perturbed problems depends of the size of the quantities $\langle \varphi_k^1 | \Delta V | \varphi_n^1 \rangle$ for any k and n .

The task of the first stage is therefore easily completed by applying (2) and (3) for $V^1 \equiv \mathcal{V}$ and $V^2 \equiv \bar{\mathcal{V}}$ and evaluating the magnitude of $\langle \varphi_k | \bar{\mathcal{V}} - \mathcal{V} | \varphi_n \rangle$. We write

$$\langle \varphi_k | \bar{\mathcal{V}} - \mathcal{V} | \varphi_n \rangle = \sum_{i=1}^{q-1} \int_{r_i}^{r_{i+1}} dr \varphi_k^*(r)(\bar{\mathcal{V}} - \mathcal{V}) \varphi_n(r). \quad (4)$$

The integrals in the sum have the same order of magnitude. The solution of the Schrödinger equation for \mathcal{V} (which is a constant in each interval) reads

$$\varphi_n(r) = A_n^i \exp(\omega_i r) + B_n^i \exp(-\omega_i r) \quad (5)$$

in the interval $[r_i, r_{i+1}]$. Here $\omega_i = [2m\hbar^{-2}(\epsilon_n - \mathcal{V})]^{1/2}$. Of course, ω_i is real or imaginary depending on whether ϵ_n is larger or smaller than \mathcal{V} . If we use the new variable $\delta = r - r_i (0 \leq \delta \leq h)$, Fig. 1 shows us that

$$\bar{\mathcal{V}} - \mathcal{V} = c \left(\delta - \frac{h}{2} \right), \quad (6)$$

where $c = [V(r_{i+1}) - V(r_i)]/h$. The integral over $[r_i, r_{i+1}]$ in (4) reads

$$J_i = c \int_0^h d\delta \varphi_k^*(r_i + \delta) \left(\delta - \frac{h}{2} \right) \varphi_n(r_i + \delta). \quad (7)$$

We now make use of the Taylor expansion of φ_j in powers of δ

$$\varphi_j(r_i + \delta) = \alpha_j^i + \frac{\delta \omega_i}{1!} \beta_j^i + \frac{\delta^2 \omega_i^2}{2!} \alpha_j^i, \quad (8)$$

which, inserted in (7) and after a little calculation, gives

$$J_i = c \frac{h^3}{12} (\alpha_k^{i*} \beta_n^i - \alpha_n^i \beta_k^{i*}). \quad (9)$$

The neglected terms are of the order $h^p (p > 3)$. In Equation (8), α_j^i and β_j^i are the values of φ_j and of its first derivative at r_i , respectively. The conclusion is that each integral of the sum in (4) gives a contribution of order h^3 . As this sum consists of $q - 1$ terms and $q - 1 = Lh^{-1}$ the result of the first stage is

$$\langle \varphi_k | \bar{\mathcal{V}} - \mathcal{V} | \varphi_n \rangle \sim h^2, \quad (10)$$

i.e., ϵ_n and $\bar{\epsilon}_n$ as well as φ_n and $\bar{\varphi}_n$ coincide except for an error $0(h^2)$.

With respect to the second stage we use once more Eqs. (2) and (3), this time for $V^1 \equiv \bar{\mathcal{V}}$ and $V^2 \equiv V$ and calculate the magnitude of the quantity $\langle \bar{\varphi}_k | V - \bar{\mathcal{V}} | \bar{\varphi}_n \rangle$. We proceed, as above,

$$\langle \bar{\varphi}_k | V - \bar{\mathcal{V}} | \bar{\varphi}_n \rangle = \sum_{i=1}^{q-1} \int_{r_i}^{r_{i+1}} \bar{\varphi}_k^*(r)(V - \bar{\mathcal{V}}) \bar{\varphi}_n(r) \quad (11)$$

and employ the well-known trapezoidal method of numerical integration,

$$\int_{x_1}^{x_2} dx f(x) = (x_2 - x_1) \frac{f(x_1) + f(x_2)}{2} - \frac{1}{12} (x_2 - x_1)^3 f''(\xi), \quad (12)$$

where the derivative is taken at a certain point $\xi \in [x_1, x_2]$. Each integral of the sum in (11) can be calculated by using (12). We observe that in our case the integrand vanishes at the ends of the integration interval as the potential difference does so; therefore,

$$\int_{r_i}^{r_{i+1}} dr \bar{\varphi}_k^*(r)(V - \bar{\mathcal{V}}) \bar{\varphi}_n(r) = -\frac{h^3}{12} \frac{d^2}{dr^2} [\bar{\varphi}_k^*(V - \bar{\mathcal{V}}) \bar{\varphi}_n]_{r=\xi}. \quad (13)$$

There are $q - 1$ such integrals in (11) and $q - 1 = Lh^{-1}$. This means that

$$\langle \bar{\varphi}_k | V - \bar{\mathcal{V}} | \bar{\varphi}_n \rangle \sim h^2. \quad (14)$$

The second stage therefore shows that $\bar{\epsilon}_n$ and E_n as well as $\bar{\varphi}_n$ and ψ_n coincide except for an error $O(h^2)$. Now by recalling the result of the first stage of the proof, one concludes that the eigenvalues and the eigenfunctions estimated by use of AM coincide, except for an error $O(h^2)$, with the exact ones, provided the approximating $\bar{\mathcal{V}}$ is the arithmetic mean value of the extreme values of V in each interval.

We now consider the truncation error in the Gordon method. We apply the formulas (2) and (3) for $V^1 \equiv V$ and $V^2 \equiv V_G$. As stated, V_G is in each interval the linear function of r which fits V as well as its derivative at the center of the interval (the line MN on Fig. 1). We have

$$\langle \psi_k | V_G - V | \psi_n \rangle = \sum_{i=1}^{q-1} \int_{r_i}^{r_{i+1}} dr \psi_k^*(r)(V_G - V) \psi_n(r). \quad (15)$$

We focus our attention on the interval $[r_i, r_{i+1}]$, denote its center by R_i , introduce the new variable $\gamma = r - R_i$ ($-h/2 \leq \gamma \leq h/2$) and make use of the Taylor expansions of V and ψ_j in powers of γ :

$$V(r) \equiv V(R_i + \gamma) = V(R_i) + \frac{\gamma}{1!} \frac{dV}{dr} \Big|_{r=R_i} + \frac{\gamma^2}{2!} \frac{d^2V}{dr^2} \Big|_{r=R_i}, \quad (16)$$

$$\psi_j(r) \equiv \psi_j(R_i + \gamma) = \psi_j(R_i) + \frac{\gamma}{1!} \frac{d\psi_j}{dr} \Big|_{r=R_i} + \frac{\gamma^2}{2!} \frac{d^2\psi_j}{dr^2} \Big|_{r=R_i}. \quad (17)$$

The neglected terms are of the order γ^p ($p > 3$). By its very definition, the potential V_G is the sum of the first and second terms in the right hand side of Eq. (16) and therefore

$$V_G - V = -\frac{\gamma^2}{2!} \frac{d^2V}{dr^2} \Big|_{r=R_i} \quad (18)$$

We introduce (17) and (18) in the integral over the interval $[r_i, r_{i+1}]$ in Eq. (15) to obtain

$$\int_{r_i}^{r_{i+1}} dr \psi_k^*(r)(V_G - V) \psi_n(r) = -\frac{h^3}{24} \psi_k^*(R_i) \psi_n(R_i) \frac{d^2V}{dr^2} \Big|_{r=R_i} \quad (19)$$

plus terms of higher order in h . Equation (19) shows that each term in the sum of the right hand side of Eq. (15) gives a contribution of order h^3 , and as there are $q - 1$ such terms and $q - 1 = Lh^{-1}$, the result is that

$$\langle \psi_k | V_G - V | \psi_n \rangle \sim h^2 \quad (20)$$

i.e., the Gordon method in which V is approximated by a linear function is a second-order method. Of course, the more accurate the approximating function V_G is, the higher is the order of the Gordon method. For example, if V_G is the sum of the first, second and third terms of the Taylor expansion, Eq. (16), the corresponding Gordon method is a third-order one.

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